

Non-perturbative construction of the Luttinger-Ward functional

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For a system of correlated electrons, the Luttinger-Ward functional provides a link between static thermodynamic quantities on the one hand and single-particle excitations on the other. The functional is useful to derive several general properties of the system as well as for the formulation of thermodynamically consistent approximations. Its original construction, however, is perturbative as it is based on the weak-coupling skeleton-diagram expansion. Here, it is shown that the Luttinger-Ward functional can be derived within a general functional-integral approach. This alternative and non-perturbative approach stresses the fact that the Luttinger-Ward functional is universal for a large class of models.

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I. INTRODUCTION

For a system of correlated electrons in equilibrium, there are several relations^{1,2,3} between static quantities which describe the thermodynamics of the system and dynamic quantities which describe its one-particle excitations. Static quantities are given by the grand potential Ω and its derivatives with respect to temperature T , chemical potential μ etc. The one-electron Green's function $\mathbf{G} = \mathbf{G}(i\omega_n)$ or the self-energy $\mathbf{\Sigma} = \mathbf{\Sigma}(i\omega_n)$, on the other hand, are dynamic quantities which yield (equivalent) information on an idealized (photoemission or inverse photoemission) excitation process.

The Luttinger-Ward functional $\hat{\Phi}[\mathbf{G}]$ provides a special relation between static and dynamic quantities with several important properties:⁴ First, the grand potential is obtained from the Luttinger-Ward functional evaluated at the exact Green's function, $\Phi = \hat{\Phi}[\mathbf{G}]$, via

$$\Omega = \Phi + \text{Tr} \ln \mathbf{G} - \text{Tr} \mathbf{\Sigma} \mathbf{G}. \quad (1)$$

Second, the functional derivative of the Luttinger-Ward functional,

$$\frac{1}{T} \frac{\delta \hat{\Phi}[\mathbf{G}]}{\delta \mathbf{G}} = \hat{\Sigma}[\mathbf{G}], \quad (2)$$

defines a functional $\hat{\Sigma}[\mathbf{G}]$ which gives the exact self-energy of the system if evaluated at the exact Green's function. The relation $\mathbf{\Sigma} = \hat{\Sigma}[\mathbf{G}]$ is independent from the Dyson equation $\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \mathbf{\Sigma}$. Third, in the non-interacting limit:

$$\hat{\Phi}[\mathbf{G}] \equiv 0 \quad \text{for } U = 0. \quad (3)$$

Finally, the functional dependence $\hat{\Phi}[\mathbf{G}]$ is completely determined by the interaction part of the Hamiltonian and independent from the one-particle part:

$$\hat{\Phi}[\mathbf{G}] \quad \text{universal}. \quad (4)$$

This universality property can also be expressed as follows: Two systems with the same interaction U but

different one-particle parameters \mathbf{t} (on-site energies and hopping integrals) in the respective Hamiltonian are described by the same Luttinger-Ward functional. Using Eq. (2), this implies that the functional $\hat{\Sigma}[\mathbf{G}]$ is universal, too.

If Ref. 4 it is shown by Luttinger and Ward that $\hat{\Phi}[\mathbf{G}]$ can be constructed order by order in diagrammatic weak-coupling perturbation theory. Φ is obtained as the limit of the infinite series of closed diagrams without any self-energy insertions and with all free propagators in a diagram replaced by fully interacting ones (see Fig. 1). Generally, this skeleton-diagram expansion cannot be summed up to get a closed form for $\hat{\Phi}[\mathbf{G}]$. So, unfortunately, the explicit functional dependence $\hat{\Phi}[\mathbf{G}]$ is actually unknown – even for the most simple Hamiltonians such as the Hubbard model.⁵ The defining properties, Eqs. (1–4), however, are easily verified.⁴

The Luttinger-Ward functional is useful for several general considerations: With the help of $\hat{\Phi}[\mathbf{G}]$ and the Dyson equation, the grand potential can be considered as a functional of the Green's function $\Omega = \hat{\Omega}[\mathbf{G}]$ or as functional of the self-energy $\Omega = \hat{\Omega}[\mathbf{\Sigma}]$, such that Ω is stationary at the physical \mathbf{G} or $\mathbf{\Sigma}$.^{4,6} This represents a remarkable variational principle which connects static with dynamic physical quantities. The Luttinger-Ward functional is also used in the microscopic derivation of some zero- or low-temperature properties of Fermi liquids as discussed in Refs. 4,7. The derivative of the functional, Eq. (2), shows the self-energy to be gradient field when considered as a functional of the Green's function, $\hat{\Sigma}[\mathbf{G}]$. This fact is related to certain symmetry properties of two-particle Green's functions as orig-

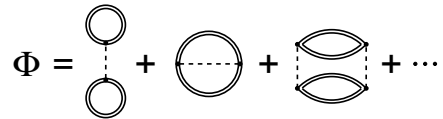


FIG. 1: Classical definition of the Luttinger-Ward functional $\hat{\Phi}[\mathbf{G}]$. Double lines: fully interacting propagator \mathbf{G} . Dashed lines: interaction U .

inally noted by Baym and Kadanoff.⁸ Furthermore, the Luttinger-Ward functional is of great importance in the construction of thermodynamically consistent approximations. So-called conserving approximations virtually start from the Luttinger-Ward functional.^{6,8} This is essential to prove these approximations to respect a number of macroscopic conservation laws. The Hartree-Fock and the random-phase approximations are well-known examples. These “classical” conserving approximations are essentially limited to the weak-coupling regime. However, the Luttinger-Ward functional can also be used to construct non-perturbative approximations. This was first realized in the context of the dynamical mean-field theory (DMFT) for lattice models of correlated electrons.^{9,10,11,12} Here, one exploits the universality of the functional, Eq. (4), to achieve an (approximate) mapping of the original lattice model onto a simpler impurity model with the same interaction part. The fact that $\hat{\Phi}[\mathbf{G}]$ is the same for a large class of systems, has recently been shown^{13,14} to be the key feature that allows to construct several non-perturbative and thermodynamically consistent approximations.^{15,16} This idea has been termed “self-energy-functional approach” (SFA).

Such general considerations remain valid as long as the Luttinger-Ward functional is well defined. This presupposes that the skeleton-diagram expansion is convergent or at least that formal manipulations of diagrammatic quantities are consistent in themselves and eventually lead to physically meaningful results. Provided that one can assure that no singular point is passed when starting from the non-interacting Fermi gas and increasing the interaction strength, this seems to be plausible. A strict proof that the skeleton-diagram expansion is well-behaved, however, will hardly be possible in most concrete situations. On the contrary, it is well known that the expansion is questionable in a number of cases, e.g. in case of a symmetry-broken state or a state that is not “adiabatically connected” to the non-interacting limit, such as a Mott insulator. The skeleton-diagram expansion may break down even in the absence of any spontaneous symmetry breaking in a (strongly correlated) state that gradually evolves from a metallic Fermi liquid. This has explicitly been shown by Hofstetter and Kehrein¹⁷ for the narrow-band limit of the single-impurity Anderson model (see Refs. 18,19 for a discussion of possible physical consequences). Generally speaking there is no strict argument available that ensures the convergence of the skeleton-diagram expansion in the strong-coupling regime.

The purpose of the present paper is to show that a construction of the Luttinger-Ward functional is possible that does not make use of the skeleton-diagram expansion. The proposed construction is based on a standard functional-integral approach and avoids the formal complications mentioned above. Thereby, one achieves an alternative and in particular non-perturbative route to the general properties of correlated electron systems derived from the functional, to the dynamical mean-field

theory as well as to the self-energy-functional approach. It should be stressed that the intended construction of the Luttinger-Ward functional requires more than a simple definition of the quantity Φ (which could trivially be achieved by using Eq. (1): $\Phi \equiv \Omega - \text{Tr} \ln \mathbf{G} + \text{Tr} \Sigma \mathbf{G}$). The task is rather to provide a functional $\hat{\Phi}[\mathbf{G}]$ with the properties Eqs. (1–4).

Previous approaches are either perturbative or cannot prove Eqs. (1–4): A construction of the Luttinger-Ward functional different from the original one⁴ has been given by Baym:⁶ The existence of $\hat{\Phi}[\mathbf{G}]$ is deduced from a “vanishing curl condition”, $\delta \Sigma(1, 1')/\delta G(2', 2) = \delta \Sigma(2, 2')/\delta G(1', 1)$, which is derived from an analysis of the functional dependence of \mathbf{G} on an arbitrary (time-dependent) external perturbation \mathbf{J} . However, an independent functional relation $\Sigma = \hat{\Sigma}[\mathbf{G}]$ is required in addition. In Ref. 6 the latter is assumed to be given by the (full or by a truncated) skeleton-diagram expansion, and consequently this approach is perturbative again.

As also shown in Ref. 6, the Green’s function in the presence of an external field \mathbf{J} can be derived from the grand potential $\hat{\Omega}[\mathbf{J}]$ as $\hat{\mathbf{G}}(\mathbf{J}) = (1/T)\delta\hat{\Omega}[\mathbf{J}]/\delta\mathbf{J}$. Using the inverse functional, $\hat{\mathbf{J}}[\mathbf{G}]$, Legendre transformation yields $\hat{\Omega}[\mathbf{G}] = \hat{\Omega}[\hat{\mathbf{J}}[\mathbf{G}]] - \text{Tr} \mathbf{G} \hat{\mathbf{J}}[\mathbf{G}]$. This (non-perturbative) functional and the Dyson equation can be used to define $\hat{\Phi}[\mathbf{G}] \equiv \hat{\Omega}[\mathbf{G}] - \text{Tr} \ln \mathbf{G} + \text{Tr} (\mathbf{G}_0^{-1} - \mathbf{G}^{-1})\mathbf{G}$. This idea is in the spirit of the effective action approach.^{20,21,22} Here, however, the problem is that the universality of $\hat{\Phi}[\mathbf{G}]$, Eq. (4), cannot be proven. The Luttinger-Ward functional constructed in this way explicitly depends on \mathbf{G}_0 and thus on the one-particle parameters \mathbf{t} .

The paper is organized as follows: The next section briefly introduces the notations and the quantities of interest. The construction of the Luttinger-Ward functional is described in Sec. III. Sec. IV gives a brief discussion of the properties of the functional and its use within the dynamical mean-field theory and the self-energy-functional approach. The results are summed up in Sec. V.

II. STATIC AND DYNAMIC QUANTITIES

Consider a system of electrons at temperature T and chemical potential μ in thermal equilibrium and let $H = H(\mathbf{t}, \mathbf{U}) = H_0(\mathbf{t}) + H_1(\mathbf{U})$ be its Hamiltonian where

$$\begin{aligned} H_0(\mathbf{t}) &= \sum_{\alpha\beta} t_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}, \\ H_1(\mathbf{U}) &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\gamma} c_{\delta}. \end{aligned} \quad (5)$$

An index α refers to an arbitrary set of quantum numbers characterizing a one-particle basis state. If N is the total particle-number operator, the grand potential of the

system is given by $\Omega_{\mathbf{t},\mathbf{U}} = -T \ln Z_{\mathbf{t},\mathbf{U}}$ where

$$Z_{\mathbf{t},\mathbf{U}} = \text{tr} \exp(-(H(\mathbf{t},\mathbf{U}) - \mu N)/T) \quad (6)$$

is the partition function. Here and in the following the dependence of all quantities on the one-particle parameters \mathbf{t} and the interaction parameters \mathbf{U} is made explicit through the subscripts.

Using a matrix notation, the free one-particle Green's function is denoted by $\mathbf{G}_{\mathbf{t},0}$. Its elements (for fixed μ) are given by:

$$G_{\mathbf{t},0,\alpha\beta}(i\omega_n) = \left(\frac{1}{i\omega_n + \mu - \mathbf{t}} \right)_{\alpha\beta}. \quad (7)$$

Here $i\omega_n = i(2n+1)\pi T$ is the n -th Matsubara frequency. The fully interacting Green's function is denoted by $\mathbf{G}_{\mathbf{t},\mathbf{U}}$. Using Grassmann variables $\xi_\alpha(i\omega_n) = T^{1/2} \int_0^{1/T} d\tau e^{i\omega_n \tau} \xi_\alpha(\tau)$ and $\xi_\alpha^*(i\omega_n) = T^{1/2} \int_0^{1/T} d\tau e^{-i\omega_n \tau} \xi_\alpha^*(\tau)$, its elements can be written as³

$$\begin{aligned} G_{\mathbf{t},\mathbf{U},\alpha\beta}(i\omega_n) &= -\langle \xi_\alpha(i\omega_n) \xi_\beta^*(i\omega_n) \rangle_{\mathbf{t},\mathbf{U}} \\ &= \frac{-1}{Z_{\mathbf{t},\mathbf{U}}} \int D\xi D\xi^* \xi_\alpha(i\omega_n) \xi_\beta^*(i\omega_n) \exp(A_{\mathbf{t},\mathbf{U},\xi\xi^*}) \end{aligned} \quad (8)$$

where

$$\begin{aligned} A_{\mathbf{t},\mathbf{U},\xi\xi^*} &= \sum_{n,\alpha\beta} \xi_\alpha^*(i\omega_n) ((i\omega_n + \mu)\delta_{\alpha\beta} - t_{\alpha\beta}) \xi_\beta(i\omega_n) \\ &\quad - \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} \int_0^{1/T} d\tau \xi_\alpha^*(\tau) \xi_\beta^*(\tau) \xi_\gamma(\tau) \xi_\delta(\tau) \end{aligned} \quad (9)$$

is the action. Finally, the self-energy is defined as

$$\Sigma_{\mathbf{t},\mathbf{U}} = \mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{G}_{\mathbf{t},\mathbf{U}}^{-1}. \quad (10)$$

The goal is to construct a functional $\hat{\Phi}_{\mathbf{U}}[\mathbf{G}]$ (where \mathbf{G} is considered as a free variable) which vanishes in the non-interacting case, $\hat{\Phi}_0[\mathbf{G}] = 0$ [Eq. (3)], which is universal, i.e. independent of \mathbf{t} [Eq. (4)], which yields $\hat{\Phi}_{\mathbf{U}}[\mathbf{G}_{\mathbf{t},\mathbf{U}}] = \Omega_{\mathbf{t},\mathbf{U}} - \text{Tr} \ln \mathbf{G}_{\mathbf{t},\mathbf{U}} + \text{Tr}(\Sigma_{\mathbf{t},\mathbf{U}} \mathbf{G}_{\mathbf{t},\mathbf{U}})$ if evaluated at the exact Green's function $\mathbf{G} = \mathbf{G}_{\mathbf{t},\mathbf{U}}$ [Eq. (1)], and the derivative of which is a functional $\hat{\Sigma}[\mathbf{G}]$ with $\hat{\Sigma}[\mathbf{G}_{\mathbf{t},\mathbf{U}}] = \Sigma_{\mathbf{t},\mathbf{U}}$ [Eq. (2)]. (Here the notation $\text{Tr} \mathbf{A} \equiv T \sum_n \sum_\alpha e^{i\omega_n 0^+} A_{\alpha\alpha}(i\omega_n)$ is used. 0^+ is a positive infinitesimal. Functionals $\hat{A} = \hat{A}[\dots]$ are indicated by a hat and should be distinguished clearly from physical quantities A .)

For the classical construction of $\hat{\Phi}_{\mathbf{U}}[\mathbf{G}]$ via the skeleton-diagram expansion (Fig. 1), these properties are easily verified: The universality of the functional [Eq. (4)] is obvious as any diagram depends on \mathbf{U} and on \mathbf{G} *only*; there is no explicit dependence on the free Green's function $\mathbf{G}_{\mathbf{t},0}$, i.e. no explicit dependence on \mathbf{t} . Since there is no zeroth-order diagram, $\hat{\Phi}_{\mathbf{U}}[\mathbf{G}]$ trivially vanishes for $\mathbf{U} = 0$ [Eq. (3)]. The functional

derivative of $\hat{\Phi}[\mathbf{G}]$ with respect to \mathbf{G} corresponds to the removal of a propagator from each of the Φ diagrams. Taking care of topological factors,^{1,4} one ends up with the skeleton-diagram expansion for the self-energy, i.e. one gets Eq. (2). Using Eq. (2), the Dyson equation (10), and $\Phi_{\mathbf{t},\mathbf{U}} \equiv \hat{\Phi}_{\mathbf{U}}[\mathbf{G}_{\mathbf{t},\mathbf{U}}]$, the μ derivative of the l.h.s and of the r.h.s of Eq. (1) are equal for any fixed interaction strength \mathbf{U} and temperature T . Namely, $(\partial/\partial\mu)(\Phi_{\mathbf{t},\mathbf{U}} + \text{Tr} \ln \mathbf{G}_{\mathbf{t},\mathbf{U}} - \text{Tr} \Sigma_{\mathbf{t},\mathbf{U}} \mathbf{G}_{\mathbf{t},\mathbf{U}}) = \text{Tr} \mathbf{G}_{\mathbf{t},\mathbf{U}}^{-1} (\partial \mathbf{G}_{\mathbf{t},\mathbf{U}} / \partial \mu) - \text{Tr} \mathbf{G}_{\mathbf{t},\mathbf{U}} (\partial \Sigma_{\mathbf{t},\mathbf{U}} / \partial \mu) = -\text{Tr} \mathbf{G}_{\mathbf{t},\mathbf{U}} = -\langle N \rangle_{\mathbf{t},\mathbf{U}} = \partial \Omega_{\mathbf{t},\mathbf{U}} / \partial \mu$. Integration over μ then yields Eq. (1). (Note that Eq. (1) holds trivially for $\mu \rightarrow -\infty$, i.e. for $\langle N \rangle_{\mathbf{t},\mathbf{U}} \rightarrow 0$ since $\Sigma_{\mathbf{t},\mathbf{U}} = 0$ and $\Phi_{\mathbf{t},\mathbf{U}} = 0$ in this limit). An equivalent derivation of Eq. (1) can be given by a coupling-constant integration.⁴

III. LUTTINGER-WARD FUNCTIONAL

The starting point is the standard functional-integral representation of the partition function as given in Ref. 3, for example: Define the functional

$$\hat{\Omega}_{\mathbf{U}}[\mathbf{G}_0^{-1}] = -T \ln \hat{Z}_{\mathbf{U}}[\mathbf{G}_0^{-1}] \quad (11)$$

with

$$\hat{Z}_{\mathbf{U}}[\mathbf{G}_0^{-1}] = \int D\xi D\xi^* \exp(\hat{A}_{\mathbf{U},\xi\xi^*}[\mathbf{G}_0^{-1}]) \quad (12)$$

and

$$\begin{aligned} \hat{A}_{\mathbf{U},\xi\xi^*}[\mathbf{G}_0^{-1}] &= \sum_{n,\alpha\beta} \xi_\alpha^*(i\omega_n) G_{0,\alpha\beta}^{-1}(i\omega_n) \xi_\beta(i\omega_n) \\ &\quad - \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} \int_0^{1/T} d\tau \xi_\alpha^*(\tau) \xi_\beta^*(\tau) \xi_\gamma(\tau) \xi_\delta(\tau). \end{aligned} \quad (13)$$

$\hat{\Omega}_{\mathbf{U}}[\mathbf{G}_0^{-1}]$ parametrically depends on \mathbf{U} . \mathbf{G}_0^{-1} is considered as a free variable. At the (matrix inverse of the) exact free Green's function, $\mathbf{G}_0^{-1} = \mathbf{G}_{\mathbf{t},0}^{-1}$, the functional yields the exact grand potential,

$$\hat{\Omega}_{\mathbf{U}}[\mathbf{G}_{\mathbf{t},0}^{-1}] = \Omega_{\mathbf{t},\mathbf{U}}, \quad (14)$$

of the system with Hamiltonian $H = H_0(\mathbf{t}) + H_1(\mathbf{U})$. Its derivative defines a functional $\hat{\mathcal{G}}_{\mathbf{U}}[\mathbf{G}_0^{-1}]$,

$$\frac{1}{T} \frac{\delta \hat{\Omega}_{\mathbf{U}}[\mathbf{G}_0^{-1}]}{\delta \mathbf{G}_0^{-1}} = - \frac{1}{\hat{Z}_{\mathbf{U}}[\mathbf{G}_0^{-1}]} \frac{\delta \hat{Z}_{\mathbf{U}}[\mathbf{G}_0^{-1}]}{\delta \mathbf{G}_0^{-1}} \equiv -\hat{\mathcal{G}}_{\mathbf{U}}[\mathbf{G}_0^{-1}], \quad (15)$$

with the property

$$\hat{\mathcal{G}}_{\mathbf{U}}[\mathbf{G}_{\mathbf{t},0}^{-1}] = \mathbf{G}_{\mathbf{t},\mathbf{U}} \quad (16)$$

which is easily verified using Eq. (8).

The strategy to be pursued is the following: $\hat{\mathcal{G}}_{\mathbf{U}}[\mathbf{G}_0^{-1}]$ is a universal (\mathbf{t} independent) functional and can be used

to construct a universal relation $\mathbf{G} = \hat{\mathbf{G}}_U[\Sigma]$ between the one-particle Green's function and the self-energy independent from the Dyson equation. Using the universal functionals $\hat{\Omega}_U[\mathbf{G}_0^{-1}]$ and $\hat{\mathbf{G}}_U[\Sigma]$, a universal functional $\hat{F}_U[\Sigma]$ is defined the derivative of which essentially yields $\hat{\mathbf{G}}_U[\Sigma]$. The Luttinger-Ward functional can then be obtained by Legendre transformation and is universal by construction.

To start with, consider the equation

$$\hat{\mathbf{G}}_U[\mathbf{G}^{-1} + \Sigma] = \mathbf{G}. \quad (17)$$

This is a relation between the variables \mathbf{G} and Σ which, for a given Σ , may be solved for \mathbf{G} . This defines a functional $\hat{\mathbf{G}}_U[\Sigma]$, i.e.

$$\hat{\mathbf{G}}_U[\hat{\mathbf{G}}_U[\Sigma]^{-1} + \Sigma] = \hat{\mathbf{G}}_U[\Sigma]. \quad (18)$$

For a given self-energy Σ , the Green's function $\mathbf{G} = \hat{\mathbf{G}}_U[\Sigma]$ is defined to be the solution of Eq. (17). From the Dyson equation (10) and Eq. (16) it is obvious that the relation (17) is satisfied for \mathbf{G} and Σ being the exact Green's function and the exact self-energy, $\mathbf{G} = \mathbf{G}_{t,U}$ and $\Sigma = \Sigma_{t,U}$, of a system with the interaction U and some set of one-particle parameters \mathbf{t} ($H = H_0(\mathbf{t}) + H_1(U)$). Hence,

$$\hat{\mathbf{G}}_U[\Sigma_{t,U}] = \mathbf{G}_{t,U}. \quad (19)$$

A brief discussion of the existence and the uniqueness of possible solutions of the relation (17) is given in Appendix A.

With the help of the functionals $\hat{\Omega}_U[\mathbf{G}_0^{-1}]$ and $\hat{\mathbf{G}}_U[\Sigma]$, a functional $\hat{F}_U[\Sigma]$ can be defined as:

$$\hat{F}_U[\Sigma] = \hat{\Omega}_U[\hat{\mathbf{G}}_U[\Sigma]^{-1} + \Sigma] - \text{Tr} \ln \hat{\mathbf{G}}_U[\Sigma]. \quad (20)$$

Using Eq. (15) one finds:

$$\begin{aligned} \frac{1}{T} \frac{\delta \hat{F}_U[\Sigma]}{\delta \Sigma} &= -\hat{\mathbf{G}}_U[\hat{\mathbf{G}}_U[\Sigma]^{-1} + \Sigma] \cdot \left(\frac{\delta \hat{\mathbf{G}}_U[\Sigma]^{-1}}{\delta \Sigma} + \mathbf{1} \right) \\ &\quad - \hat{\mathbf{G}}_U[\Sigma]^{-1} \cdot \frac{\delta \hat{\mathbf{G}}_U[\Sigma]}{\delta \Sigma}, \end{aligned} \quad (21)$$

and, using Eq. (18),

$$\frac{1}{T} \frac{\delta \hat{F}_U[\Sigma]}{\delta \Sigma} = -\hat{\mathbf{G}}_U[\Sigma]. \quad (22)$$

So $\hat{\mathbf{G}}_U[\Sigma]$ can be considered as the gradient of the (scalar) self-energy functional $\hat{F}_U[\Sigma]$. Therewith, the Legendre transform of $\hat{F}_U[\Sigma]$ can be constructed:

$$\hat{\Phi}_U[\mathbf{G}] = \hat{F}_U[\hat{\Sigma}_U[\mathbf{G}]] + \text{Tr}(\hat{\Sigma}_U[\mathbf{G}] \mathbf{G}). \quad (23)$$

Here $\hat{\Sigma}_U[\mathbf{G}]$ is the inverse of the functional $\hat{\mathbf{G}}_U[\Sigma]$. The functional can be assumed to be invertible (locally) provided that the system is not at a critical point for a phase transition (see also Ref. 13). Eq. (23) defines the Luttinger-Ward functional.

IV. DISCUSSION

A. Properties of the Luttinger-Ward functional

The properties of the Luttinger-Ward functional, Eqs. (1–4), can be verified easily: Eqs. (10), (14), (19) and (20) imply

$$\hat{F}_U[\Sigma_{t,U}] = \Omega_{t,U} - \text{Tr} \ln \mathbf{G}_{t,U}, \quad (24)$$

and with $\hat{\Sigma}_U[\mathbf{G}_{t,U}] = \Sigma_{t,U}$ the evaluation of the Luttinger-Ward functional at $\mathbf{G} = \mathbf{G}_{t,U}$ yields

$$\Phi_{t,U} \equiv \hat{\Phi}_U[\mathbf{G}_{t,U}] = \Omega_{t,U} - \text{Tr} \ln \mathbf{G}_{t,U} + \text{Tr}(\Sigma_{t,U} \mathbf{G}_{t,U}), \quad (25)$$

i.e. Eq. (1). From Eqs. (22) and (23), one immediately has:

$$\frac{1}{T} \frac{\delta \hat{\Phi}_U[\mathbf{G}]}{\delta \mathbf{G}} = \hat{\Sigma}_U[\mathbf{G}], \quad (26)$$

i.e. Eq. (2). In the limit $U = 0$, the functionals $\hat{\mathbf{G}}_{U=0}[\Sigma]$ and $\hat{F}_{U=0}[\Sigma]$ are ill-defined (the domain of the functionals shrinks to a single point, $\Sigma = 0$, see Appendix A). However, from Eq. (25), one directly has $\Phi_{U=0}[\mathbf{G}_{t,0}] = 0$ for any \mathbf{t} [see Eq. (3)] since $\Sigma_{t,0} = 0$ and $\Omega_{t,0} = \text{Tr} \ln \mathbf{G}_{t,0}$ (a proof for the latter can be found in Ref. 4). Finally, the universality of $\hat{\Phi}_U[\mathbf{G}]$, Eq. (4) is obvious as the definition (23) of the Luttinger-Ward functional involves the universal (\mathbf{t} independent) functionals $\hat{F}_U[\Sigma]$ and $\hat{\Sigma}_U[\mathbf{G}]$ only.

B. Variational principle

Using the Legendre transform of the Luttinger-Ward functional $\hat{F}_U[\Sigma]$, one may define

$$\hat{\Omega}_{t,U}[\Sigma] = \text{Tr} \ln \frac{1}{\mathbf{G}_{t,0}^{-1} - \Sigma} + \hat{F}_U[\Sigma]. \quad (27)$$

The functional derivative is easily calculated:

$$\frac{1}{T} \frac{\delta \hat{\Omega}_{t,U}[\Sigma]}{\delta \Sigma} = \frac{1}{\mathbf{G}_{t,0}^{-1} - \Sigma} - \hat{\mathbf{G}}_U[\Sigma]. \quad (28)$$

The equation

$$\hat{\mathbf{G}}_U[\Sigma] = \frac{1}{\mathbf{G}_{t,0}^{-1} - \Sigma} \quad (29)$$

is a (highly non-linear) conditional equation for the self-energy of the system $H = H_0(\mathbf{t}) + H_1(U)$: Eqs. (10) and (19) show that it is satisfied by the exact self-energy $\Sigma = \Sigma_{t,U}$. Note that the l.h.s of (29) is independent of \mathbf{t} but depends on U (universality of $\hat{\mathbf{G}}_U[\Sigma]$), while the r.h.s is independent of U but depends on \mathbf{t} via $\mathbf{G}_{t,0}^{-1}$. The obvious problem of finding a solution of Eq. (29) is that

there is no closed form for the functional $\hat{G}_U[\Sigma]$. Solving Eq. (29) is equivalent to a search for the stationary point of the grand potential as a functional of the self-energy:

$$\frac{\delta \hat{\Omega}_{t,U}[\Sigma]}{\delta \Sigma} = 0. \quad (30)$$

Similarly, one can also construct a variational principle using the Green's function as the basic variable, $\delta \hat{\Omega}_{t,U}[\mathbf{G}]/\delta \mathbf{G} = 0$.

C. Dynamical mean-field theory

The dynamical mean-field theory^{9,10,11,12} basically applies to lattice models of correlated electrons with on-site interactions such as the Hubbard model,⁵ for example. The DMFT aims at an approximate solution of Eq. (29) and is based on two ingredients:

(i) It is important to note that the Luttinger-Ward functional $\hat{\Phi}_U[\mathbf{G}]$ is the same for the lattice (e.g. Hubbard) model and for an impurity model (single-impurity Anderson model). Actually a (decoupled) set of impurity models has to be considered – one impurity model with the according local interaction at each site of the original lattice. This ensures that the interaction (U) term is the same as in the lattice model. (In case of translational symmetry the a priori different impurity models can be assumed to be equivalent). As U is the same in the lattice and in the impurity model, the Luttinger-Ward functional, as well as $\hat{G}_U[\Sigma]$, is the same.

(ii) Let the lattice model be characterized by one-particle parameters t and the impurity model by parameters t' . The fundamental equation (29) for the lattice model would then be solved by the exact self-energy $\Sigma_{t,U}$. As an ansatz for an approximate solution Σ of Eq. (29), the self-energy is assumed to be local within the DMFT and to be representable as the exact self-energy of the impurity model for some parameters t' :

$$\Sigma = \Sigma_{t',U}. \quad (31)$$

The universality of the Luttinger-Ward functional (i) and the local approximation for the self-energy (ii) are sufficient to derive the DMFT: Inserting the ansatz (31) into Eq. (29) yields a conditional equation for the one-particle parameters of the impurity model t' . The l.h.s becomes $\hat{G}_U[\Sigma_{t',U}] = \mathbf{G}_{t',U}$, i.e. the exact Green's function of the impurity model, while the r.h.s reads $(\mathbf{G}_{t,0}^{-1} - \Sigma_{t',U})^{-1}$. The resulting equation for the parameters t' can be fulfilled only locally, i.e. by equating the local elements of the respective Green's functions at the impurity and the original site respectively:

$$(\mathbf{G}_{t',U})_{\text{loc}} = \left(\frac{1}{\mathbf{G}_{t,0}^{-1} - \Sigma_{t',U}} \right)_{\text{loc}}. \quad (32)$$

This is the so-called self-consistency equation of the DMFT.¹²

This consideration can be seen as an independent and, in particular, non-perturbative re-derivation of the DMFT which supplements known approaches such as the cavity method.¹²

D. Self-energy-functional approach

The universality of the Luttinger-Ward functional or of its Legendre transform $\hat{F}_U[\Sigma]$ is central to the recently developed self-energy-functional approach.^{13,14} The SFA is a general variational scheme which includes the DMFT as a special limit. The idea is to take as an ansatz for the self-energy of a model $H = H_0(t) + H_1(U)$ the exact self-energy $\Sigma_{t',U}$ of a so-called reference system $H' = H_0(t') + H_1(U)$ that shares with the original model the same interaction part. The parameters t' of the one-particle part are considered as variational parameters to search for the stationary point of the grand potential as a functional of the self-energy. This means to insert the ansatz $\Sigma = \Sigma_{t',U}$ into the general expression (27) and to solve the Euler equation $\partial \hat{\Omega}_{t,U}[\Sigma_{t',U}]/\partial t' = 0$, i.e.:

$$\frac{\partial}{\partial t'} \left(\text{Tr} \ln \frac{1}{\mathbf{G}_{t,0}^{-1} - \Sigma_{t',U}} + \hat{F}_U[\Sigma_{t',U}] \right) = 0 \quad (33)$$

for t' . If the search for the optimum set of one-particle parameters t' was unrestricted, the approach would be exact in principle as the Euler equation would then be equivalent with the Euler equation (29) of the general variational principle Eq. (30).

A restriction of the space of variational parameters becomes necessary to evaluate the quantity $\hat{\Omega}_{t,U}[\Sigma_{t',U}]$ which, in general, is impossible as a closed form for the functional $\hat{F}_U[\Sigma]$ is not known. With a proper restriction, however, the reference system H' can be made accessible to an exact (numerical) solution which allows to derive the exact grand potential and the exact Green's function of the system H' . Therewith, making use of the universality of $\hat{F}_U[\Sigma]$ and using Eqs. (23) and (25) for the reference system,

$$\hat{F}_U[\Sigma_{t',U}] = \Omega_{t',U} - \text{Tr} \ln \mathbf{G}_{t',U}. \quad (34)$$

Note that this implies that an exact evaluation of $\hat{F}_U[\Sigma]$ is possible for self-energies of a exactly solvable reference system with the same interaction part as the original one. Using this result in Eq. (33), one obtains:

$$\frac{\partial}{\partial t'} \left(\Omega_{t',U} + \text{Tr} \ln \frac{1}{\mathbf{G}_{t,0}^{-1} - \Sigma_{t',U}} - \text{Tr} \ln \mathbf{G}_{t',U} \right) = 0, \quad (35)$$

which can be evaluated to fix t' and therewith the optimal self-energy and grand potential (see Refs. 13,14,15,16 for details and concrete examples).

E. Luttinger's theorem

Finally, the role of the Luttinger-Ward functional in the derivation of general properties of correlated electron systems shall be discussed. As an important example, the Luttinger theorem⁴ is considered. For a translationally invariant system, the theorem states that in the limit $T \rightarrow 0$ the average particle number is equal to the volume enclosed by the Fermi surface in \mathbf{k} space:

$$\langle N \rangle = V_{\text{FS}}. \quad (36)$$

The Fermi surface is defined by the set of \mathbf{k} points in the first Brillouin zone that satisfies $\mu - \eta_{\mathbf{k}} = 0$ where $\eta_{\mathbf{k}}$ are the eigenvalues of the matrix $\mathbf{t} + \Sigma(\omega)$ at vanishing excitation energy $\omega = 0$. Hence, to formulate the Luttinger theorem, one obviously has to presuppose that there is a Fermi surface at all, i.e. that $\Sigma(\omega = 0)$ is Hermitian.²⁵ The original proof of the theorem⁴ is perturbative as it makes use of the skeleton-diagram expansion. A non-perturbative proof, based on topological considerations, was proposed recently²³ and is based on the assumption that the system is a Fermi liquid.

To discuss the Luttinger theorem in the present context, consider the following shift transformation of the Green's function

$$\mathbf{S}^{(z)} \mathbf{G}(i\omega_n) = \mathbf{G}^{(z)}(i\omega_n) = \mathbf{G}(i\omega_n + iz) \quad (37)$$

with $z = 2\pi kT$ and k integer (z is a bosonic Matsubara frequency). $\mathbf{S}^{(z)}$ is a linear and unitary transformation. The shift transformation leaves the functional integral Eq. (11) unchanged:

$$\widehat{\Omega}_U[\mathbf{S}^{(z)} \mathbf{G}_0^{-1}] = \widehat{\Omega}_U[\mathbf{G}_0^{-1}]. \quad (38)$$

To verify this invariance, one has to note that the shift of the Matsubara frequencies in \mathbf{G}_0^{-1} by z can be transformed into a shift $\omega_n \rightarrow \omega_n - z$ in the Grassmann numbers:

$$\xi_\alpha(i\omega_n) \rightarrow \xi_\alpha(i\omega_n - iz). \quad (39)$$

In imaginary-time representation this shift is equivalent with the multiplication of a phase:

$$\xi_\alpha(\tau) \rightarrow e^{-iz\tau} \xi_\alpha(\tau), \quad \xi_\alpha^*(\tau) \rightarrow e^{iz\tau} \xi_\alpha^*(\tau). \quad (40)$$

This, however, leaves the functional integral unchanged as the transformation Eq. (39) or Eq. (40) is linear and the Jacobian is unity. Note that antiperiodic boundary conditions $\xi_\alpha(\tau = 1/T) = -\xi_\alpha(\tau = 0)$ are respected for a bosonic shift frequency z .

Denoting $\Omega_{\mathbf{t},U}(z) \equiv \widehat{\Omega}_U[\mathbf{S}^{(z)} \mathbf{G}_{\mathbf{t},0}^{-1}]$, Eq. (38) states that $\Omega_{\mathbf{t},U}(z) = \Omega_{\mathbf{t},U}(0)$. Following the steps in the construction of the Luttinger-Ward functional in Sec. III, one easily verifies that this implies $\Phi_{\mathbf{t},U}(z) = \Phi_{\mathbf{t},U}(0)$ where $\Phi_{\mathbf{t},U}(z) \equiv \widehat{\Phi}_U[\mathbf{S}^{(z)} \mathbf{G}_{\mathbf{t},U}]$. For the Legendre transform, one has $F_{\mathbf{t},U}(z) = F_{\mathbf{t},U}(0)$ where $F_{\mathbf{t},U}(z) \equiv$

$\widehat{F}_U[\mathbf{S}^{(z)} \Sigma_{\mathbf{t},U}]$. Now, in the limit $T \rightarrow 0$, z becomes a continuous variable. Hence,

$$\frac{d}{dz} \lim_{T \rightarrow 0} F_{\mathbf{t},U}(z) = 0. \quad (41)$$

If the limit and the derivative can be interchanged,

$$\frac{d}{dz} \lim_{T \rightarrow 0} F_{\mathbf{t},U}(z) = \lim_{T \rightarrow 0} \frac{d}{dz} F_{\mathbf{t},U}(z), \quad (42)$$

Eqs. (24) and (41) imply

$$-\lim_{T \rightarrow 0} \frac{d\Omega_{\mathbf{t},U}(z)}{dz} = -\lim_{T \rightarrow 0} \frac{d\text{Tr} \ln \mathbf{S}^{(z)} \mathbf{G}_{\mathbf{t},U}}{dz}. \quad (43)$$

The z dependence of the grand potential is the same as its μ dependence, and thus $-(d/dz)\Omega_{\mathbf{t},U}(z = 0) = -\partial\Omega_{\mathbf{t},U}/\partial\mu = \langle N \rangle$. The evaluation of the r.h.s in Eq. (43) is straightforward and can be found in Ref. 4, for example. It turns out that at $z = 0$ the r.h.s is just the Fermi-surface volume V_{FS} .

Consequently, the non-perturbative construction of the Luttinger-Ward functional allows to reduce the proof of the Luttinger theorem to the proof of Eq. (42). This, however, requires certain assumptions on the regularity of the $T \rightarrow 0$ limit which are non-trivial generally.

V. SUMMARY

To summarize, the present paper has shown that the Luttinger-Ward functional can be constructed within the framework of functional integrals under fairly general assumptions. In particular, there is no need for an adiabatic connection to the non-interacting limit and no expansion in the interaction strength as was required in the original approach of Luttinger and Ward.⁴ The construction merely assumes the very existence of the functional integral over Grassmann fields, i.e. the existence of the Trotter limit, for the representation of the partition function.

It is well known that the Luttinger-Ward functional can be employed for different purposes, some of which have been discussed here: The functional is used to derive some general properties of correlated electron systems, such as the Luttinger theorem. It allows to formulate a variational principle involving a thermodynamical potential as a functional of the Green's function or the self-energy and thereby provides a unique and thermodynamically meaningful link between static and dynamic quantities which is helpful for interpretations and for the construction of approximations. An independent derivation of the dynamical mean-field is possible using the special properties of the Luttinger-Ward functional and the universality of the functional in particular. The latter is of central importance in the context of the self-energy-functional approach which is a general framework to construct thermodynamically consistent approximations.

Referring to the standard definition of the Luttinger-Ward functional that is based on the weak-coupling skeleton-diagram expansion, the above-mentioned and any further considerations based on the functional and its unique properties meet with criticism when applied to strongly correlated, non-Fermi liquid or symmetry-broken states. This is exactly the point where the presented non-perturbative construction of the Luttinger-Ward functional is useful.

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APPENDIX A

As the relation (17) is highly non-linear, the existence and the uniqueness of possible solutions have to be discussed:

Take U to be fixed and assume that the self-energy

given is the exact self-energy of a system $H = H_0(t) + H_1(U)$ with some hopping parameters t . So the self-energy Σ is assumed to be given from the space \mathcal{S}_U of t representable self-energies $\mathcal{S}_U \equiv \{\Sigma | \Sigma = \Sigma_{t,U}, t \text{ arbitrary}\}$ (U fixed). With the help of Eq. (16) it is then obvious that the exact Green's function of this system, $G = G_{t,U}$, solves Eq. (17) as the Dyson equation (10) shows that $G_{t,U}^{-1} + \Sigma_{t,U}$ is the exact free Green's function of this system. Concluding, one has $\hat{G}_U[\Sigma_{t,U}] = G_{t,U}$, and thus the existence of a solution is guaranteed on the space \mathcal{S}_U . Note that it is very convenient to consider \mathcal{S}_U as the domain of the functional $\hat{G}_U[\Sigma]$ since this ensures the correct analytical and causal properties of the variable Σ .

Under the functional $\hat{G}_U[\Sigma]$ the space \mathcal{S}_U is mapped onto the space \mathcal{G}_U of t representable Green's functions $\mathcal{G}_U \equiv \{G | G = G_{t,U}, t \text{ arbitrary}\}$ (U fixed). Generally, the map $\hat{G}_U : \mathcal{S}_U \rightarrow \mathcal{G}_U$ is not unique.¹³ Hence, the uniqueness of the functional $\hat{G}_U[\Sigma]$ must be enforced by a proper restriction of the range \mathcal{G}_U , i.e. of the solution set of Eq. (17). The considerations in Secs. III and IV, however, are unaffected and hold for any choice of the range, see also the related discussion in Ref. 13.

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- ¹ A. A. Abrikosow, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, New Jersey, 1964).
 - ² A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).
 - ³ J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Addison-Wesley, Redwood City, 1988).
 - ⁴ J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).
 - ⁵ J. Hubbard, Proc. R. Soc. London A **276**, 238 (1963).
 - ⁶ G. Baym, Phys. Rev. **127**, 1391 (1962).
 - ⁷ J. M. Luttinger, Phys. Rev. **119**, 1153 (1960).
 - ⁸ G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961).
 - ⁹ W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
 - ¹⁰ A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992).
 - ¹¹ M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992).
 - ¹² A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
 - ¹³ M. Potthoff, Euro. Phys. J. B **32**, 429 (2003).
 - ¹⁴ M. Potthoff, Euro. Phys. J. B **36**, 335 (2003).
 - ¹⁵ M. Potthoff, M. Aichhorn, and C. Dahnken, Phys. Rev. Lett. **91**, 206402 (2003).
 - ¹⁶ C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, and M. Potthoff, preprint cond-mat **0309407** (2003).
 - ¹⁷ W. Hofstetter and S. Kehrein, Phys. Rev. B **59**, R12732 (1999).
 - ¹⁸ S. Kehrein, Phys. Rev. Lett. **81**, 3912 (1998).
 - ¹⁹ G. Kotliar, Euro. Phys. J. B **11**, 27 (1999).
 - ²⁰ S. Y. Savrasov and G. Kotliar, preprint cond-mat **0106308** (2001).
 - ²¹ S. Y. Savrasov and G. Kotliar, preprint cond-mat **0308053** (2003).
 - ²² A. Georges, preprint cond-mat **0403123** (2004).
 - ²³ M. Oshikawa, Phys. Rev. Lett. **84**, 3370 (2000).
 - ²⁴ J. K. Freericks and V. Zlatić, Rev. Mod. Phys. **75**, 1333 (2003).
 - ²⁵ For systems without Fermi surface, there is no Luttinger theorem. A nice example is given by the Falicov-Kimball model in infinite dimensions, see Ref. 24.